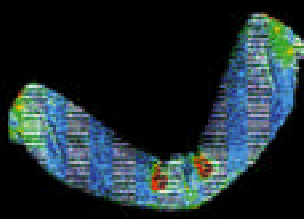
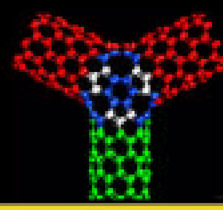
Nanotechnology Research at NASA Ames

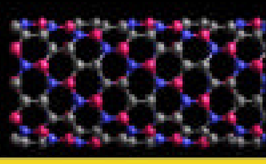
M. Meyyappan, T.R. Govindan, and Harry Partridge
NASA Ames Research Center
Moffett Field, CA 94035



Nano-mechanics/materials

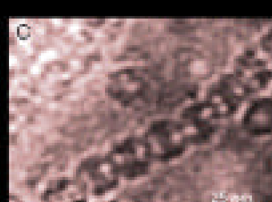


Carbon based electronics

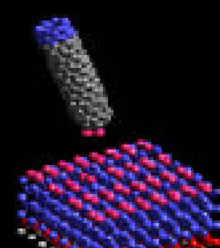


BxCyNz Nanotubes

Nanotube - Motor



Protein Nanotubes



Nano-synthesis/etching

Nanotechnology Research at NASA Ames

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Abstract

This article provides an overview of nanotechnology research at NASA Ames Research Center and covers current results in the areas of carbon nanotube (CNT) growth and characterization, nanotubes in scanning probe microscopy, biosensors, protein nanotubes, atomic chain electronics, computational nanotechnology, quantum device simulation, and computational optoelectronics.

I. Introduction

NASA Ames started an Integrated Product Team (IPT) on Devices and Nanotechnology in FY 97 to conduct basic research in the emerging field of nanotechnology as well as in semiconductor device physics, computational electronics and optoelectronics, and computational chemistry in materials processing. Advanced miniaturization is a key thrust area to enable new science and exploration missions for which ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed. Revolutions in electronics and computing will allow reconfigurable, autonomous, "thinking" spacecraft. Nanotechnology presents a whole new spectrum of opportunities to build device components and systems for entirely new, bold space architectures such as networks of ultrasmall probes on planetary surfaces, micro-rovers that drive, hop, fly and burrow, and collection of microspacecraft making a variety of measurements.

The Ames group has grown to a level of about forty scientists and Table 1 lists those who are involved in nanotechnology research and contributed to the material presented in this article. The research focus, summarized in Table 2, covers a wide range of subjects: carbon nanotube (CNT) synthesis, characterization, sensor development, application of CNT in atomic force microscopy (AFM), development of quantum device simulator, computational optoelectronics, atomic chain electronics, and bacteriorhodapsin (BR) based holographic data storage. This article provides selected results in the above areas. A complete current publication list from the Ames group as well as descriptive project summaries can be found in the IPT website http://www.ipt.arc.nasa.gov. This website also features a nanotechnology gallery containing videos and images [1].

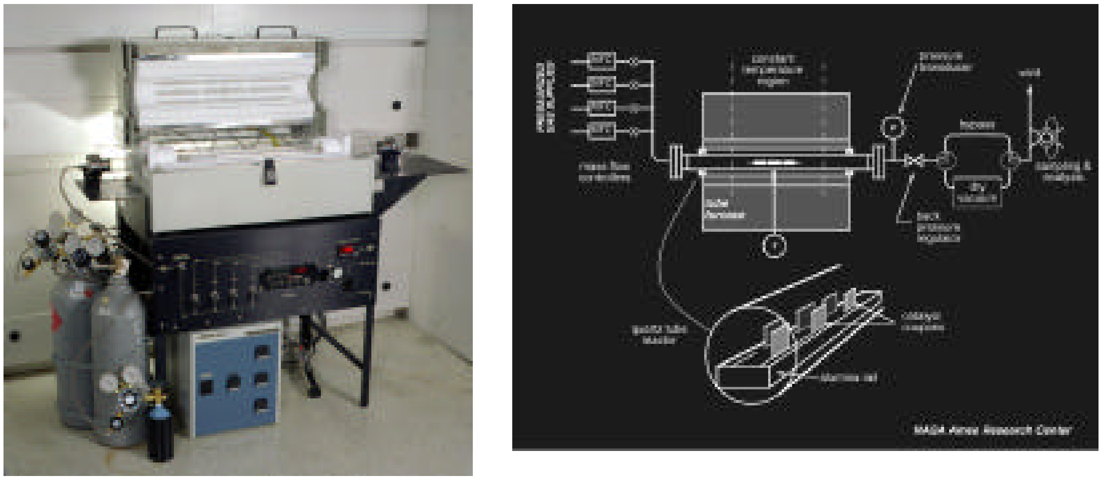


Fig. 1. Ames CVD reactor for nanotube growth

II. Carbon Nanotube: Experimental Work

CNTs have been primarily grown by laser ablation [2] and carbon arc techniques [3] by various research groups across the world. Both approaches produce single wall CNT in small quantities scraped off the cooler walls of the tube. Ames operates two chemical vapor deposition (CVD) reactors to grow nanotubes on substrates. CVD, a workhorse in silicon microelectronics, is ideally suited to grow nanotubes on patterned substrates if one is interested in investigating nanoelectronic devices or sensors. Figure 1 shows a schematic of our CVD reactor which can hold several small substrates. The feed gas may be CO or some hydrocarbon gas, and typical growth temperatures for multiwall carbon nanotubes is 500-800 deg. C. The furnace is capable of isothermal operation (± 1 deg.) over the entire ~ 2 ft. length. The CNT growth is catalyzed by transition metals such as nickel, iron or cobalt and we use a mixture of these metals. The catalyst mixture can be applied to the substrate by solution chemistry followed by heating, or direct sputtering of various metals. Parameters controlling growth appear to be numerous: nature of feedgas and composition, flow rate, temperature, type of catalyst, catalyst preparation technique, and substrate material. To date, no research group has been able to control CNT diameter or chirality. Since the number of variables involved is very large, a combinatorial chemistry approach is being used currently in our group for CNT synthesis. Figure 2 shows a bundle of multiwall CNT grown by CVD. Current efforts also include growth on patterned substrates and single wall nanotubes.

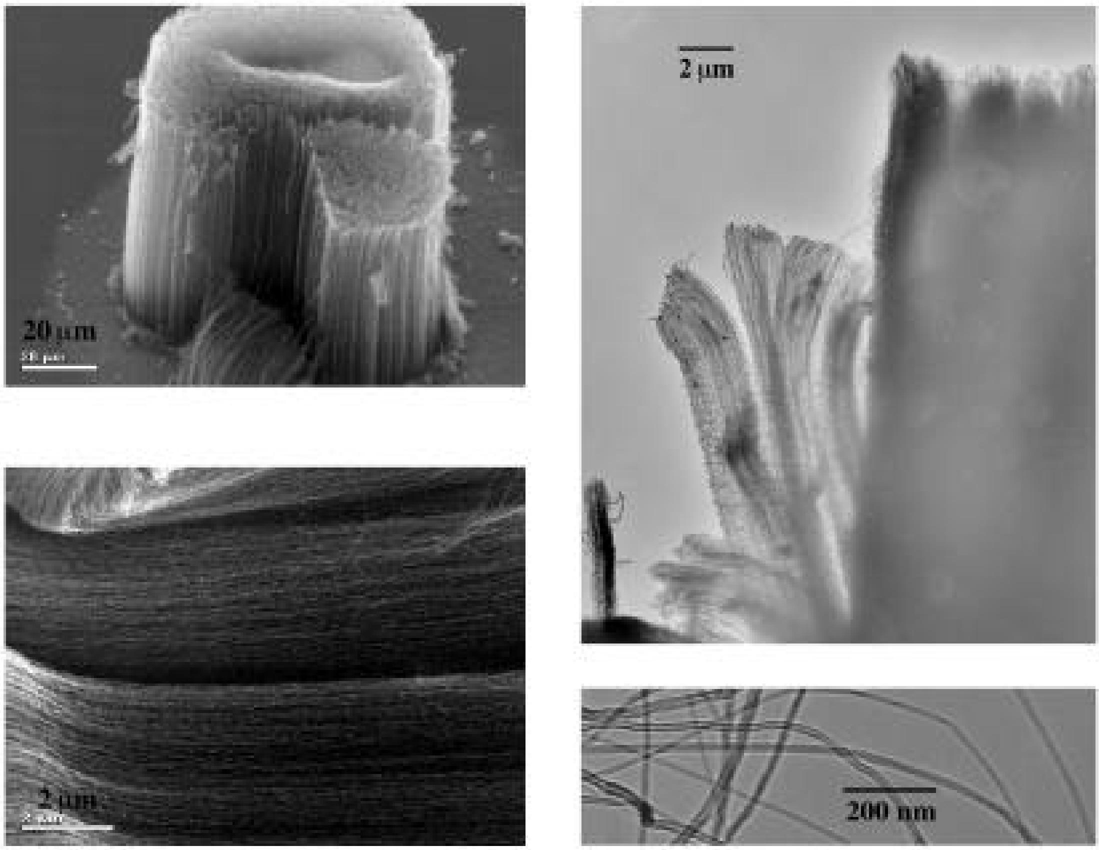
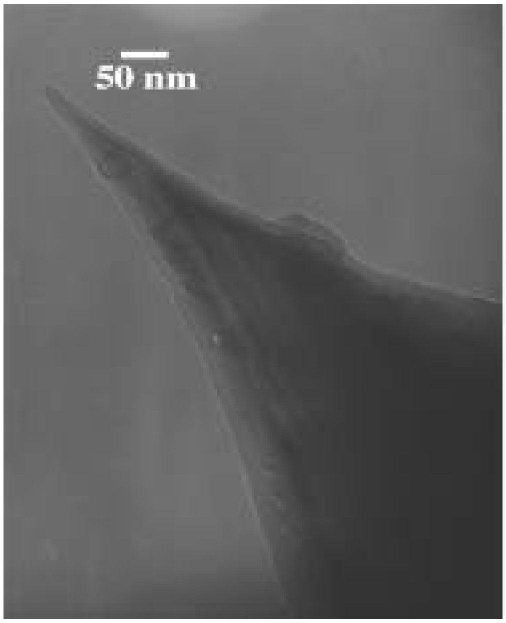


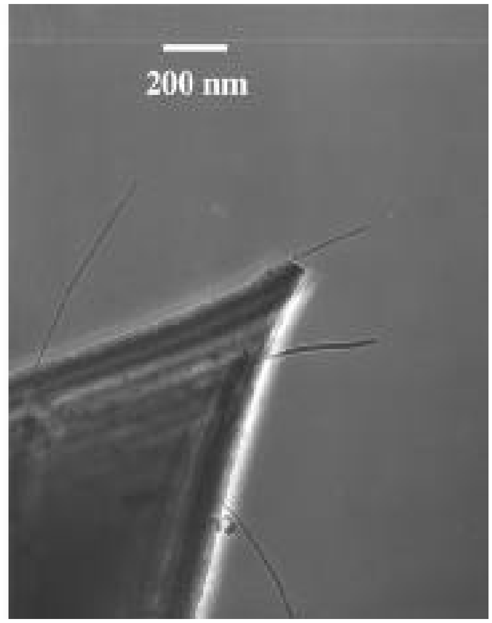
Fig. 2. Carbon nanotubes grown by CVD

CNT is an ideal tip for use in AFM [4] since it is robust and can be just a few nanometers in diameter. However, attaching a CNT to the tip of a cantilever can be arduous. Our group has been able to use CVD to directly grow nanotubes on the AFM cantilever. Figure 3 shows an example of the effort. Typically, nanotubes appear on the sides of the pyramidal cantilever as well, but these can be readily eliminated leaving only the nanotube at the tip. The AFM with nanotube tip is currently used to image and study simulated Mars dust as well as Mars meteorite ALH84001. Figure 4 shows a comparison of simulated Mars dust imaged with conventional micromachined silicon tip and CNT tip. The CNT tip - only a few nanometers in diameter - is able to offer extraordinary resolution in imaging the dust whereas the larger silicon tip results in artificial triangular shape for all the particles under focus in Fig. 4. In addition, the robustness of CNT provides long lasting tips in contrast to the quick wearing of silicon tips. It is noted that a

CNT tip in AFM has been successfully used in nanolithography [4] in a collaborative work between Stanford University and Ames. Future work in this direction would include metrology applications (for example, a profilometer) and CNT based nanomanipulator.



TEM Micrograph of Electro-deposited Catalyst on Tip of AFM Cantilever

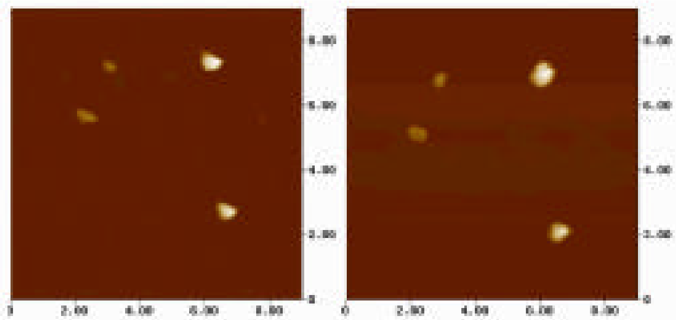


TEM Micrograph of Shortened NT Synthesized by CVD

Fig. 3. Nanotube tip directly grown on AFM cantilever.

Storage of hydrogen in nanotubes has been studied by many research groups and the results to date have been controversial. The work at Ames has used single wall nanotube (SWNT) samples from the Rice and UCLA groups and found only about 1% hydrogen uptake at atmospheric pressure and various temperatures. This result correlates well with unpublished observations from other groups we know. The nanotubes used at Ames were about 1.5 nm in diameter. It is believed that the ends were closed in as-received samples, and no attempt was made to open the ends. Further work currently in this area includes simulation to understand mechanisms, experimentation with large diameter CNTs and pursuing chemisorption routes.

A major area of focus in CNT applications at Ames is development of biosensors for cancer diagnostics. This work, conducted in collaboration with National Cancer Institute, involves development of a prototype biosensor catheter that permits detection of specific oligonucleotide sequences that serve as molecular signatures of cancer cells. The biosensor will be tested in vitro using tissue samples from patients with chronic myelogeneous leukemia and acute promyelocytic leukemia, neoplastic diseases for which molecular signatures have been well characterized. The CNT-based biosensor technology under development for cancer diagnostics will also be adapted for use in astrobiology missions, and related plans are underway. A critical element of this technology involves the ability to functionalize the tip of a nanotube array with (a monolayer of) probe molecules which is an active area of research at Ames.



Mars dust imaged with standard silicon tip (left) and a single wall carbon nanotube tip (right). The nanotube tip was reported to be 50-70 nm long and 2-3 nm diameter. original images: simars4.017(left) and tmars4.014

Fig. 4.   Tapping mode AFM images of simulated mars dust on mica using different tips

III. Nanotubes: Theory and Simulation

Extensive investigations using computational simulations on the electronics, mechanical and other properties of nanotubes have been undertaken by the Ames nanotechnology group. Carbon nanotubes exhibit remarkable mechanical properties, for example, a Young's modulus of over 1 TPa and tensile strength of about 200 GPa. They also have been unique electronic properties in that a CNT, based on its diameter and helicity, can either metallic or semiconducting. It is interesting to explore the coupling between the mechanical and electronic properties. Figure 5 shows sample results from a combination of molecular mechanics, dynamics, and tight binding simulations. The bandgap, normalized by the hopping parameter (3.1 eV) and a dimensionless radius R/Ro, is plotted against strain for various chiral tubes. For reference, the bandgap of a (10, 0) tube at 0% strain is 1 eV whereas the bandgap of silicon is 1.11 eV. The metallic (5, 5) tube shows no variation in bandgap under tension or compression whereas other tubes show varying degree of change. The slope itself depends on the modulus of (n-m, 3) where n and m are used to define the chirality. Within each color coded group in Fig. 5, the magnitude of the change depends on the chiral angle. For example, the bandgap changes more rapidly for a (10, 0) tube compared to a (6, 5) tube. In general, there are three transitions seen in Fig. 5. The first is metal-semiconductor transition, for example, the (9, 0) tube at 1% strain. Next, the change in bandgap with strain (slope) changes sign due to quantum number change, for example, the (10, 0) tube at 10% strain. Finally, another transition is seen when the slope changes sign again due to mechanical relaxation, for example, the (10, 0) tube at 18% strain. The critical strain, defined at the transition point due to quantum number change, varies inversely with tube diameter (not shown here) which can be verified experimentally. Further details can be found in ref. 5 which also describes the effects of torsional strain on the bandgap. Reference 6 describes the effect of bending on the electronic properties.

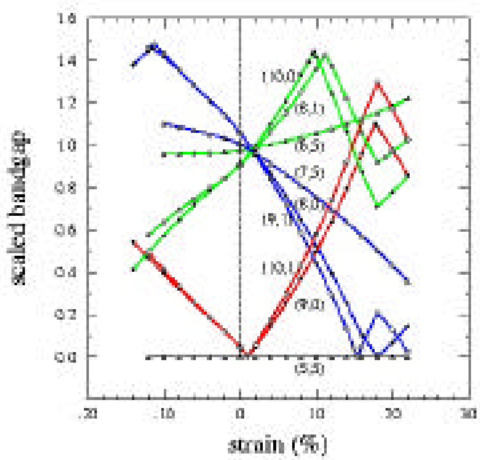


Fig. 5. Effect of strain on bandgap. Legend: n - m = 3q + 1, n - 3 = 3q, n - 3 = 3q - 1, where n, m and q are integers.

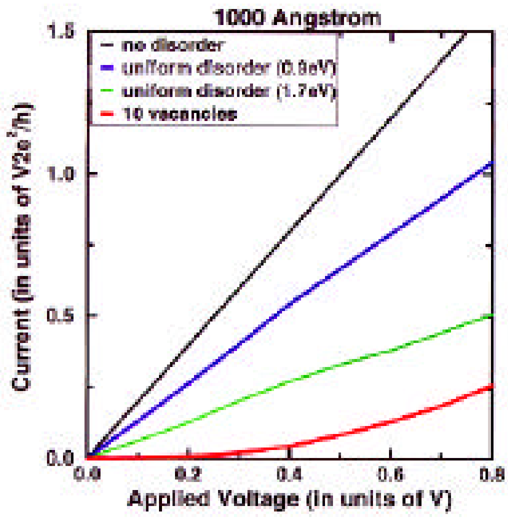


Fig. 6. Effect of disorder on CNT conductance.

A CNT is expected to be an ideal quantum wire. Ballistic transport through a nanotube would yield a low bias resistance of 6KΩ. The best measurements to date for single wall nanotubes have been shown to be in the range of 20-50 KΩ. The main reasons for the observed low conductance are defects and Bragg reflection. Theoretical work studying the effect of disorders and reflection on conductance has been carried out. Figure 6 shows computed conductance for nanotubes with uniform disorders and vacancies. Uniform disorder in CNT does not significantly affect conductance. In contrast, vacancy-type defects cause significant backscattering resulting in a conductance degradation. Further details can be found in ref. 7. Another important aspect in CNT-based electronics is the role of contacts, and theoretical investigations have been carried out to study how a carbon nanotube couples to simple metals. For good coupling, the K_f for metals must be greater than $4\pi/3a_0$ ($1.7\,\mathring{A}^{-1}$ for graphite). The value of K_f for Al and Au are 1.75 and 1.21 respectively and graphite does not couple to these metals. For armchair nanotubes, this value is only $0.85\mathring{A}^{-1}$ and coupling to simple metals is very good. The armchair tube also couples better than zigzag tubes to metal. The computations show an increase in transmission with the length of the contact, as seen in experiments. Details of this study can be found in ref. 8.

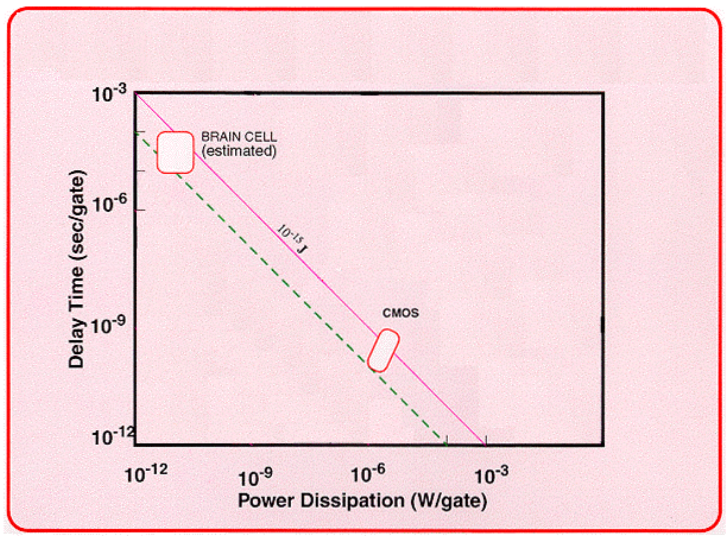


Fig. 7. Power dissipation per gate as a function of delay time

The unique electronic properties of CNT have led to the fabrication of the first CNT-based field effect transistor by research groups at IBM and Delft University. The CNT-FET consisted of a SWNT in contact with source and drain contacts and was modulated by a gate on the backside. The device operated at room temperature. In ref. [9], Yamada provides a theoretical analysis of the experimental data by incorporating one-dimensional quantum effects in the nanotube channel. He concludes that the lack of saturation in drain current as a function of drain voltage is an indication of channel carrier transport dominated by weak-localization and the electrode metal-nanotube contact influences subthreshold channel conductance vs. gate voltage. Yamada recommends a reduction in gate oxide thickness to increase the transistor gain.

While attempts to fabricate a CNT-FET are necessary first steps and allow exploration of fundamental issues and ultimate possibilities, it is critical, at this early stage, to pay attention to nanoelectronic circuit and architectures. Simple miniaturization of a CMOS-like device may not be appropriate for future nanoelectronics. Figure 7 shows switching time vs. power consumption per gate for a CMOS architecture. As device feature size and switching delay time decrease, the power consumption per gate goes up significantly and a CNT-based CMOS-like architecture is likely to face serious problems. It is interesting to note in the same plot that the brain, admittedly orders of magnitude slower, consumes significantly less power. It is possible to develop novel architectural concepts based on the unique properties of CNT, particularly metal-semiconductor, semiconductor-semiconductor, and heterojunctions [10, 11]. Figure 8 shows nanoscale tunnel junctions for transistors which were constructed by introducing topological defects such as five (pentagon) and seven (heptagon) member rings in an otherwise all six (hexagon) based CNT [11]. Heterojunctions based on partial chemical functionalization and/or substitutional doping may also be possible. In addition to CNT, the Ames group has also been investigating boron nitride nanotubes [12], for electronics and structural applications.

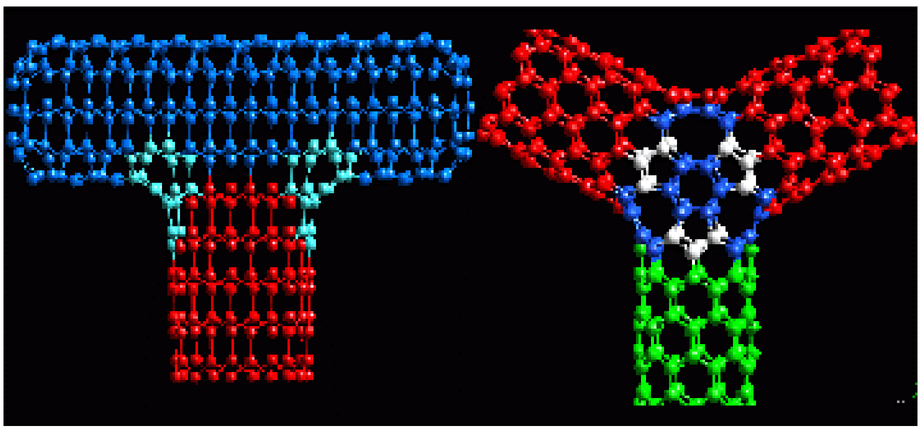
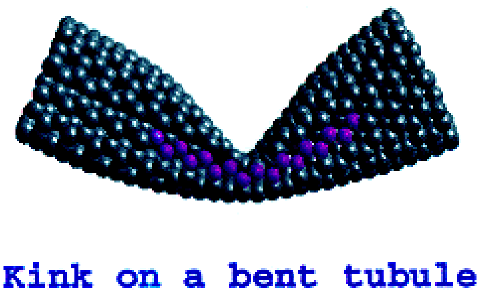


Fig. 8. Carbon nanotube "T" and "Y" junctions

The remarkable mechanical properties of CNT are by now well known. Applications to high strength composites require extensive investigation to understand the behavior of CNT under various conditions. Nanoplasticity of SWNTs under uniaxial compression was studied using generalized tight-binding molecular dynamics, and ab initio electronic structure method [13]. The bonding geometry collapses from a graphitic (sp^2) to a localized diamond like (sp^3) reconstruction under axial compression. Videoclips of this can be seen on the web under ref. [1]. The computed critical stress of about 153 GPa and the shape of the resulting plastic deformation agree well with experimental observations. Based on measurements of electrical conductivity, the thermal conductivity of SWNT has been speculated to be in the range of 1750-5800 W/m.K. which would put it in a class with CVD grown diamond. Molecular dynamics simulation at Ames has shown [14] a thermal conductivity in the range of 1000-2500 W/m.K for a (10, 10) nanotube at temperatures 100-500 deg. K. Note that this high thermal conductivity is only in the axial direction with K values in the radial direction being small. Further work is in progress to compute thermal conductivity of multiwall tubes.



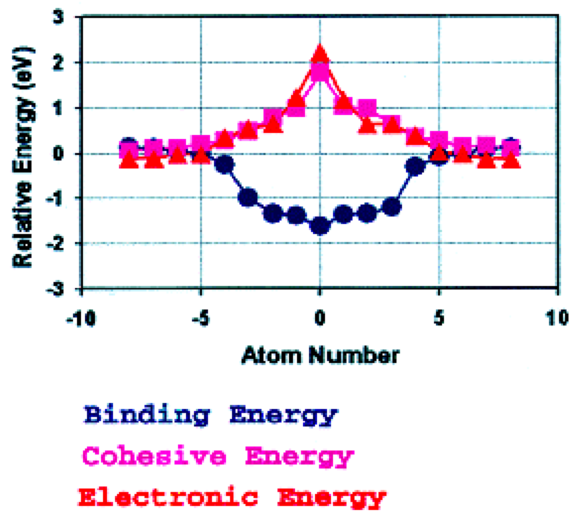


Fig. 9. Energies at various sites in a bent nanotube

Several contemplated applications for CNT require functionalization of the nanotubes (both the tip and the sidewall). Indeed, recent efforts at Rice University showed that functionalization with F atoms decreases the conductivity of nanotubes. Ames theoretical work predicts an enhanced chemical reactivity at regions of local conformational strain on the nanotubes [15]. Nanotubes which are bent or twisted show enhanced reactivity for specific sites near the distortions, as shown in Figure 9 which plots the binding energy, cohesive energy, and electronic energy for several highlighted atoms in a bent-tube. Preliminary verification of this prediction was provided by Rod Ruoff of Washington University where nanotubes laid over a V-ridge substrate were selectively attacked by nitric acid only at the sites distorted by the ridge [15].

The unique properties of CNT make it an attractive candidate for several nanotechnology innovations. The Ames computational nanotechnology researchers have designed a CNT-based nanogear [16, 17] shown in Fig. 10. Benzyne molecules bonded to the side of the nanotube form teeth while the nanotube forms the body about which the gear rotates. Computer simulations show that stable rotations of the driven gear are possible with the forced rotations of the powered gear. Videoclips of the nanogear rotation can be found in the website in ref. 1. The use of CNT tips in an AFM-based lithography and other applications were mentioned in section I. The possibility of nanoscale etching using CNT tips has been investigated through molecular dynamic simulations. Selective atomic scale etching as well as indentation of silicon surfaces by CNT tips (mounted in an AFM) have been shown to be possible [18]. Parallelization of an array of tips has the potential to revolutionize future generation lithography. The website in ref. 1. contains videoclips of CNT etching and indentation. The possibility of storing data using H and F atoms to signify 0 and 1 bits has also been theoretically investigated [19, 20]. These atoms are sufficiently small that the interaction between adjacent data atoms on a silicon surface is small. Reference 19 speculates on how such a memory device might be constructed. A method then must be devised to differentiate between H and F atoms unambiguously. A suggested mechanism is to have a probe that is attractive toward one atom and repulsive to the other and ref. 20 discusses the suitability of a Sc atom and electron-rich pyridine molecule as probes (to be attached to the tip of a CNT). This type of chemical storage of data is capable of 10^{15} bytes/cm^2 storage density. Parallelization of tips again can overcome speed-related problems.

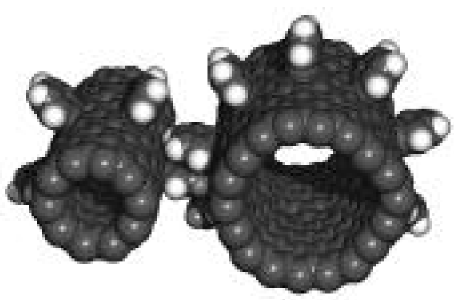


Fig. 10. A CNT-based nanogear with benzyne molecules bonded as teeth

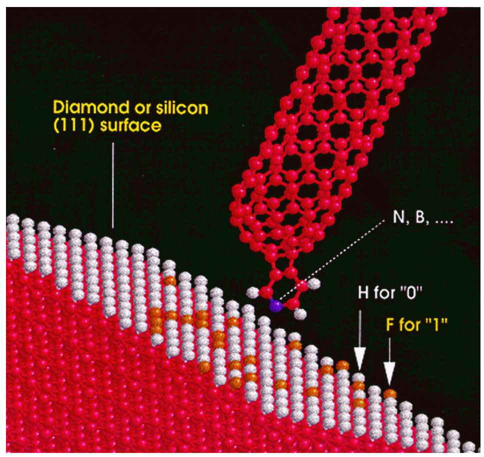


Fig. 11. Chemical data storage with H and F atoms as 0 and 1 to be read by a functionalized CNT tip.

IV. Protein Nanotubes

Jonathan Trent and coworkers at NASA Ames have been studying "heat shock protein 60" (HSP60) in organisms living at high temperatures, the so-called "thermophiles." The

HSP60 can be purified from cells as a double-ring structure consisting of 16-18 subunits. The Ames group has recently discovered that the double-rings can be induced to self-assemble into tubes and then the tubes associate to form filaments [21]. The protein nanotubes shown in Fig. 12 are about 15 nm in diameter and several microns long. The nanotubes are stable up to near 100°C, depending on the pH. Figure 13 shows an STM image of these rings and nanotubes. Currently, several applications for these protein nanotubes are being explored.

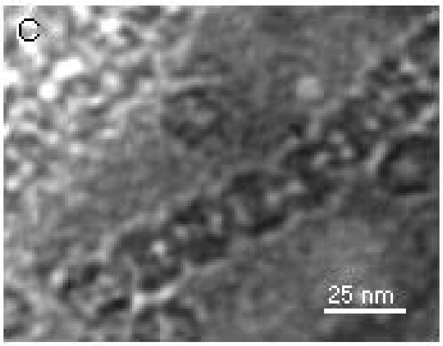


Fig. 12. Protein nanotubes

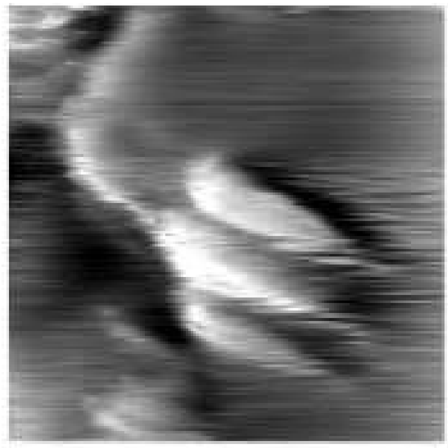


Fig. 13. STM image of a HSP60 protein nanotube

V. Bacteriorhodapsin Based Data Storage

Memory is a commodity for which there will always be an ever-increasing demand. The need for higher capacity and fast access data storage media and systems - both for various NASA Enterprises and the commercial sector - is well known. Timucin and coworkers at Ames have been investigating a holographic optical data storage system based on the biological photochrome bacteriorhodapsin (BR), a retinal protein molecule found in the purple cell membrane of the organism *halobacterium salinarium*. Figure 14 shows the BR photocycle. The anticipated performance of the system is 3-D multiplexed storage with greater than 10^{11} bits/cm^3 volume density, 100-500 Gbytes in a CD-sized platter (which represents 20-100 times DVD capacity) and 100-500 Mbits/sec 2-D parallel (associative) readout rate. The BR meets several desirable properties for a storage medium: response to visible light and hence, optically recordable and erasable; offers high resolution (~5000 lines/mm) and low fatigue (>10^8 cycles); real-time holography; respectable dynamic range, low scattering; and chemically stable with extended storage lifetimes. High quality BR films have been fabricated and techniques to improve sensitivity and lifetime have been identified. Extensive modeling and simulation has been undertaken to understand mechanisms and resolve key issues. The photocycles of BR have been experimentally characterized and storage demonstration has been made.

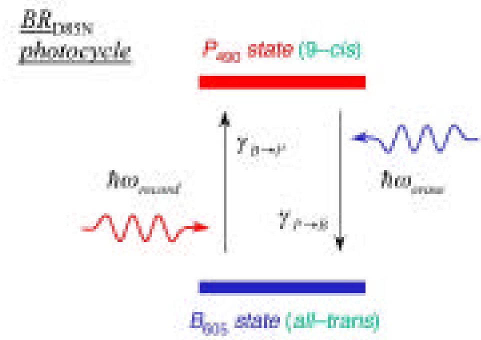


Fig. 14. Photocycle of bacteriolrhodopsin

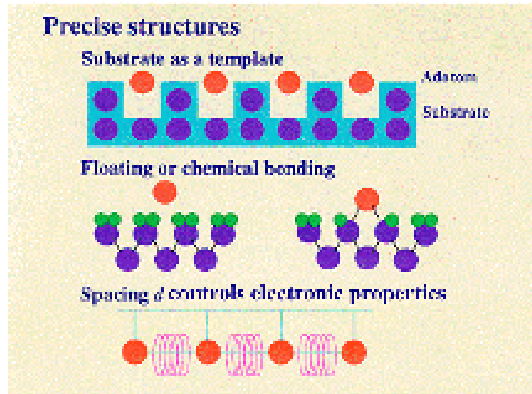


Fig. 15. Atomic chain electronics

VI. Atomic Chain Electronics

The current generation CMOS and other devices have a feature scale of 0.25 µm or above and their properties are uniform, predictable and controllable. As the venture continues into sub 0.1 µm levels, the mesoscopic devices are expected to have nonuniform characteristics and unreliable device performance. For example, the number of impurity atoms in a 50 nm gate device would be so small that the randomness in doping would disappear, which will pose serious limits on integration. This has inspired T. Yamada of Ames to investigate atomic chain electronics which are precise structures of adatoms placed on an atomically regulated surface using atom manipulation technology [see Fig. 15]. Note that significant capabilities in atom manipulation technology exist today which would allow placing atoms along a line on a chosen substrate using a scanning tunnel microscope tip acting as a tweezer. The innovative concept of atomic chains is worth pursuing as a candidate for building future electronics devices.

The lattice constant of an atomic chain determines the band structure and Fermi energy; this allows electronic property engineering. Theoretical predictions show that a Si chain is always metallic while a Mg chain is semiconducting. These determinations are for chains without a substrate, i.e. "floating in air." Recent efforts on chemical bonding scheme have shown that the adatom chain properties are influenced by the substrate surface, characterized by the number of chemical bonds to the substrate atom per adatom. This determines the following to be semiconducting: group IV adatoms with two chemical bonds each and group III adatoms with one chemical bond each. Unintentional doping would result due to change transfer between adatoms and substrate atoms. A doping scheme for semiconductor chains has also been developed. A tight-binding theory with universal parameters was undertaken to address this issue and the results show that the doping can be achieved with an atomic-modulation scheme, i.e. to place the dopant atoms beside the chain periodically. Group I atoms would be the choice for donors and Group VII atoms for acceptors. Future work involves contact schemes and evaluation of device performance. Further details can be found in ref. [22-24].

VII. Computational Electronics

The main trends in device miniaturization are relentless downscaling of CMOS technology and exploration of molecular devices. Future generation smaller and faster devices are of critical importance to powerful onboard computing, autonomous "thinking" spacecraft, and petaflop computing initiative. Modeling and simulation not only provides an understanding of how these devices work, but also can serve as a design tool in developing new generation devices. In submicron devices under consideration, the electron wavelength is comparable to device dimensions and the transit time becomes comparable to scattering time. Under these conditions, classical propagators fail. The Ames Computational Electronics group has developed a multidimensional quantum device simulator based on a Nonequilibrium Green's Function (NEGF) approach. Figure 16 shows a 25 nm-MOSFET studied using this simulator along with contours of electron density.

VIII. Computational Optoelectronics

Optoelectronics is a major enabling technology for the tera-era information technology. Information transmission, processing, and storage are key areas of active research in optoelectronics. Ames has a significant computational optoelectronics activity in progress. The goal is to develop comprehensive modeling and large scale simulation capability for studying and design of quantum optoelectronics devices. Vertical cavity surface-emitting laser (VCSEL) is one of the most advanced and smallest semiconductor laser with light coming vertically out of the semiconductor wafer surface (see Fig. 17). It can be integrated with transistors in peta-flop computing with VCSEL-based optical interconnects, interprocessor communication, multi-gigabit Ethernet, high throughput image processing and virtual reality, and biological and chemical detection of molecules of interest in astrobiology and other space applications. Ames has developed a comprehensive model and simulation of VCSELs in 2-D space and time domain thus allowing detailed investigation of transverse modes. Figure 17 shows snapshots of computed laser intensity for a VCSEL. Other investigations include ultrafast modulation of semiconductor lasers [25] for high speed communication and compact and coherent THz sources [26].

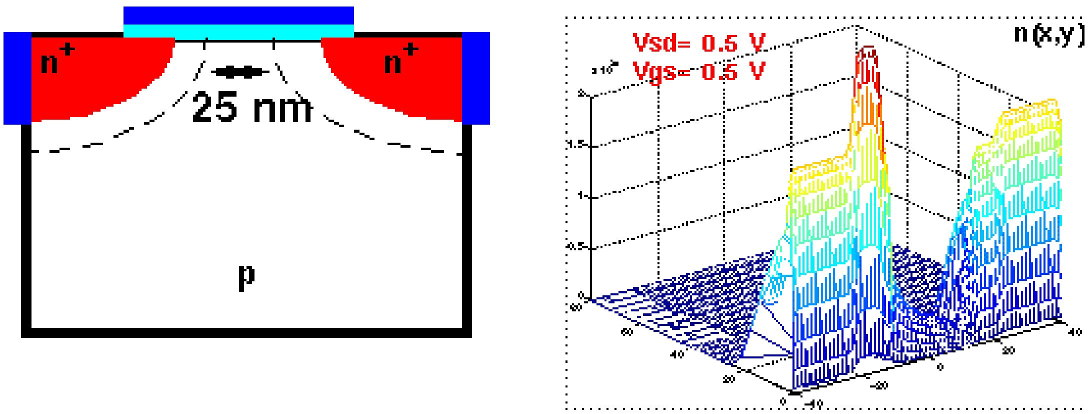


Fig. 16. Electron density contours for a 25 nm CMOS computed using a NEGF approach.

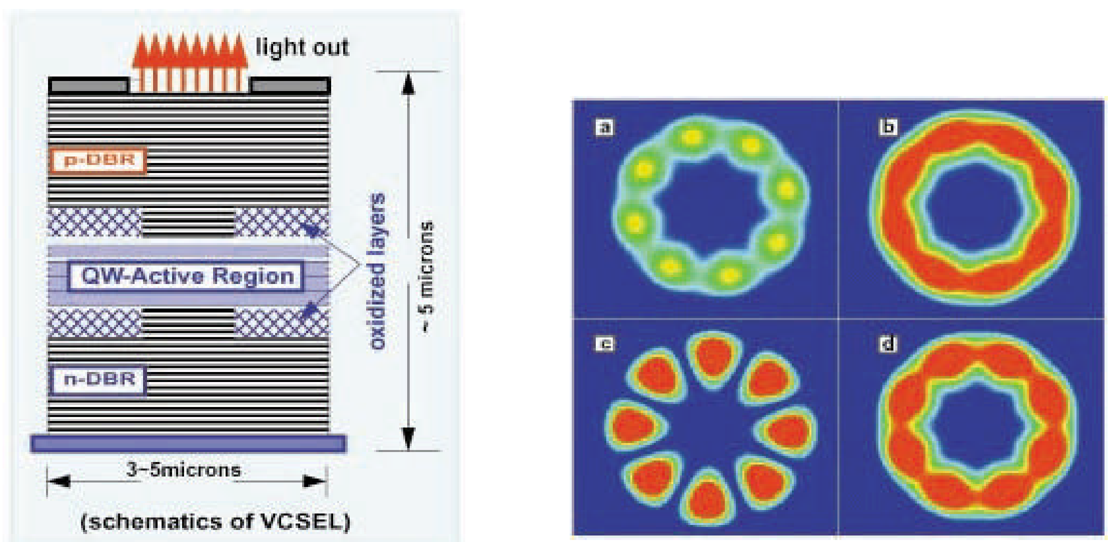


Fig. 17. 2 Dimensional VCSEL simulation showing laser intensity.

IX. Concluding Remarks

Nanotechnology - in its various forms such as nanoelectronics, nanoelectromechanical systems, ultrasmall and highly sensitive sensors, multifunctional materials, biologically inspired materials, systems and architectures, and possibly many others scientists have not yet thought of - is expected to play a strong and critical role in future space transportation and exploration. NASA Ames IPT on Devices and Nanotechnology has been conducting innovative research in this emerging field to meet Agency's future needs. Ames has particularly a strong program in carbon nanotubes and the research activities cover growth, characterization, CNT-based sensors, AFM-based applications, and computational simulation. Future plans include continued expansion of laboratory facilities and capabilities to meet the goal of developing prototype nanodevices and sensors. Alternatives to CNT such as protein nanotubes with unique applications are also being explored.

Atomic chain electronics, another innovative concept in nanoelectronics, appears to be promising and capabilities exist in various laboratories across the world today to create an atomic chain transistor. Excellence in computational sciences has long been a tradition at Ames, and Ames organizations such as Numerical Aerodynamic Simulation (NAS) Division and Computational Chemistry Branch have led the way in numerous subjects of interest to the Agency. In that tradition, a strong program in computational nanotechnology, computational quantum electronics, and computational quantum optoelectronics is being pursued. The vision for this program is to develop highly integrated and intelligent simulation environment that facilitates the rapid development and validation of future generation of electronic, photonic, and other devices, and sensors as well as materials and processes through virtual prototyping at multiple levels of fidelity.

Acknowledgement

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Table 1.

NASA Ames Nanotechnology Research Team		
Carbon Nanotubes/Sensors	Toshi Yamada	***Collaboration***
M.P. Anantram	Liu Yang	David Blake
Charlie Bauschlicher	***Protein Nanotubes***	Exobiology Branch, ARC
Alan Cassell	Johnathan Trent	John Marshall
Lance Delzeit	Lance Delzeit	Exobiology Branch, ARC
Fedor Dzegilinko	Bishun Khare	John Hines
John Finn	***Computational Electronics***	Sensor 2000, ARC
Jie Han	M.P. Anantram	David Loftus, M.D.
Ann Hermone	Bryan Biegel	Stanford Medical Center
Rich Jaffe	T.R. Govindan	Prof. K.R. Sridhar,
Jim Kaysen	Alexi Svizhenko	Prof. S. Manne
Shoudan Liang	***Computational Optoelectronics***	U. of Arizona
Cattien Nguyen	Cun-Zheng Ning	
Deepak Srivastava	Peter Goorjian	
Ramsey Stevens	Jianzhong Li	
Sunita Verma	Ansheng Liu	
	Holographic Data Storage	
	Dogan Timucin	

Table 2.

Research Focus

Nanotechnology • Nanotubes - Controlled, patterned growth of CNT - Large scale production of CNT - Hydrogen storage in nanotubes - CNT-based biosensor for cancer diagnostics - Functionalization of nanotubes - AFM study of Mars dust - AFM study of Mars meteorite - CNT-based sensors for astrobiology - Protein nanotubes: growth and applications - Reactor/Process Modeling of CNT growth - Computational investigation of electronic, mechanical and other properties of CNT - Transport in CNT, Nanoelectronics - BN nanotubes, structure and properties - Design of CNT-based mechanical components	• Chemical Storage of Data • Atomic Chain Electronics • Bacteriorhodapsin based holographic data storage ***Computational Electronics, Computational Optoelectronics*** - Development of multidimensional quantum simulators to design ultrasmall semiconductor devices - Development of semiclassical methods with quantum correction terms - Investigation of device technologies suitable for petaflop computers - Modeling of optoelectronics devices, VCSEL, THz modulation - Optical interconnect modeling